Intoduction to Optimization

Computer Graphics CMU 15-462/15-662

Last time: physically-based animation

- Use dynamics to drive motion
- **Complexity from simple models**
 - **Technique: numerical integration**
 - formulate equations of motion
 - take little steps forward in time
 - general, powerful tool
 - **Today: numerical optimization**
 - another general, powerful tool
 - basic idea: "ski downhill" to get a better solution
 - used everywhere in graphics (not just animation)
 - image processing, geometry, rendering, ...



What is an optimization problem?

- Natural human desire: find the best solution among all possibilities (subject to certain constraints)
- E.g., cheapest flight, shortest route, tastiest restaurant ... Has been studied since antiquity, e.g., isoperimetric problem:

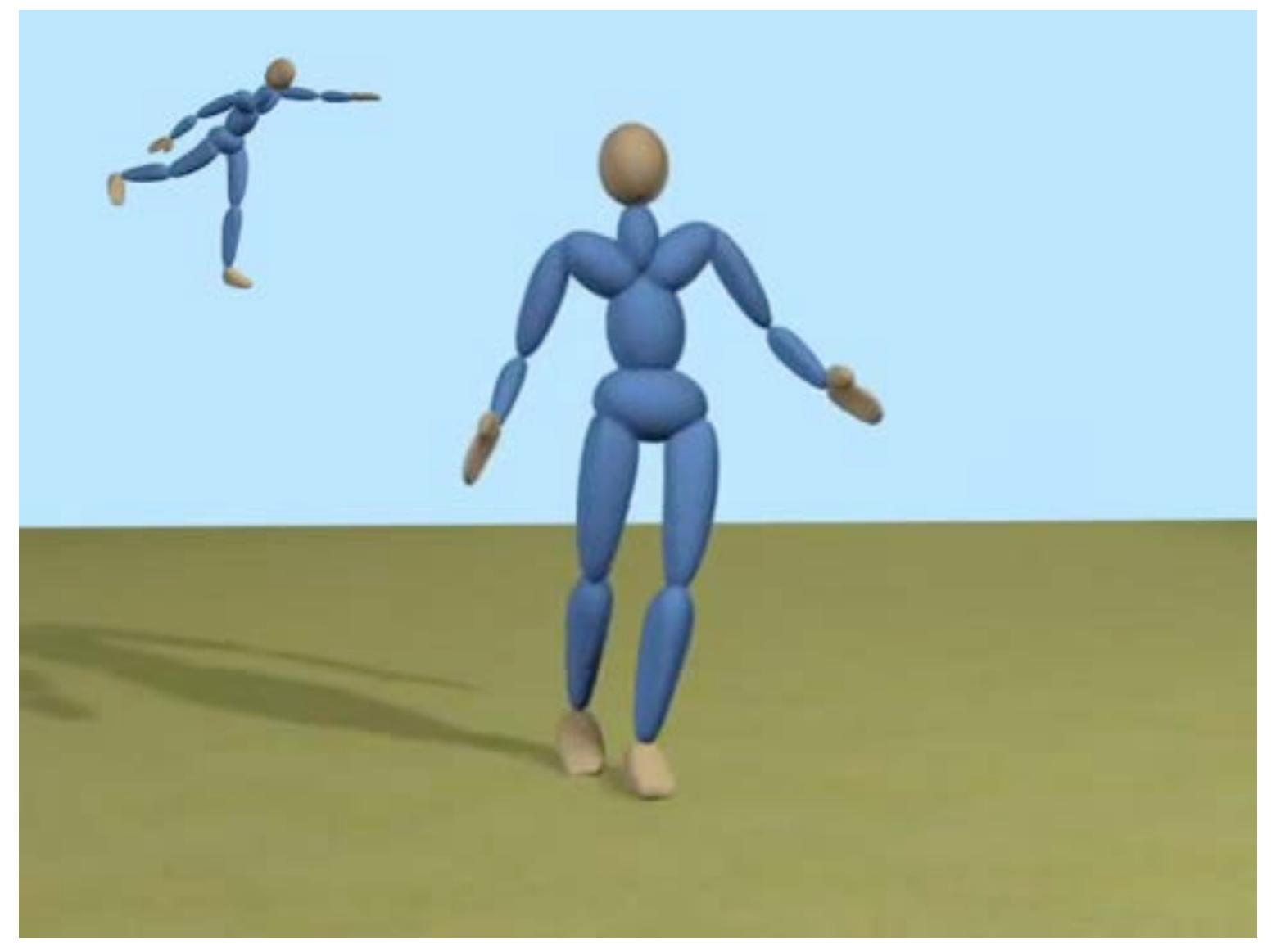
"The first optimization problem known in history was practically solved by Dido, a clever Phoenician princess, who *left her Tyrian home and emigrated to North Africa, with all* her property and a large retinue, because her brother Pygmalion murdered her rich uncle and husband Acerbas, and plotted to defraud her of the money which he left. On landing in a bay about the middle of the north coast of Africa she obtained a grant from Hiarbas, the native chief of the district, of as much land as she could enclose with an oxhide. She cut the ox-hide into an exceedingly long strip, and succeeded in enclosing between it and the sea a very valuable territory on which she build Carthage."

—Lord Kelvin, 1893

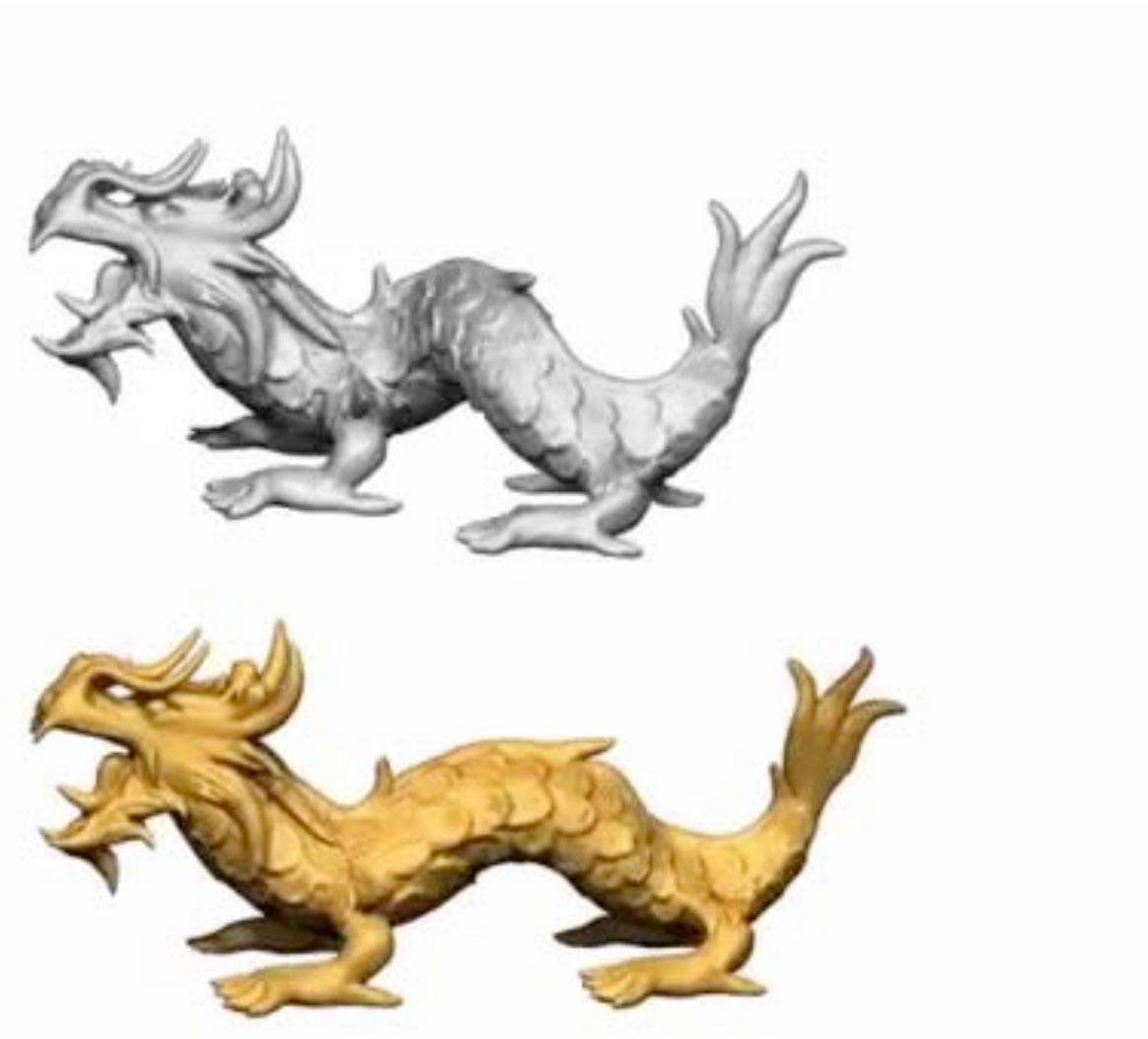
"Obvious" solution is a circle...

CARTHAGE

...but wait, what about the coastline?

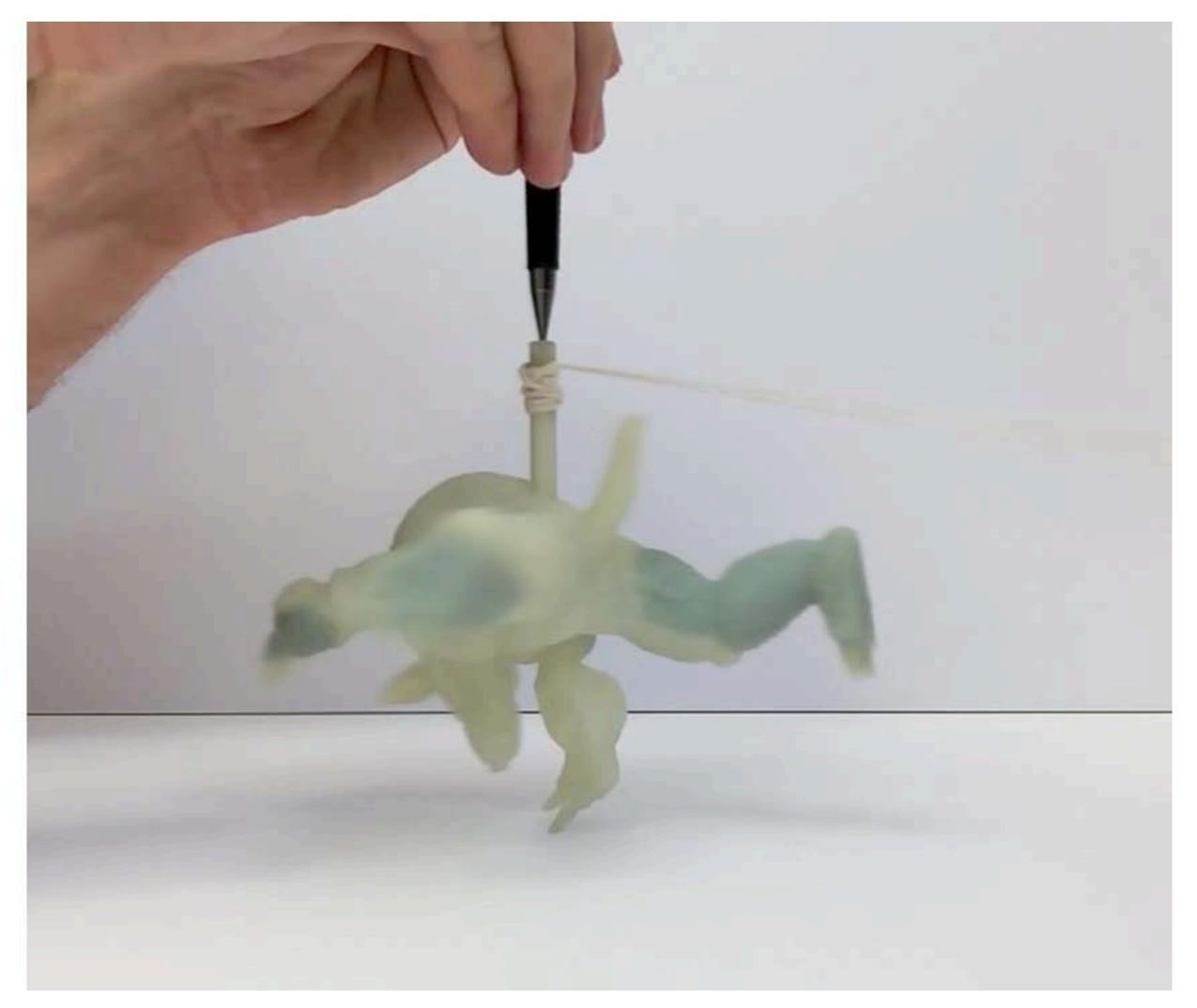


Sumit Jain, Yuting Ye, and C. Karen Liu, "Optimization-based Interactive Motion Synthesis"



Niloy J. Mitra, Leonidas Guibas, Mark Pauly, "Symmetrization"

optimized result





Moritz Bächer, Emily Whiting, Bernd Bickel, Olga Sorkine-Hornung, "Spin-It: Optimizing Moment of Inertia for Spinnable Objects"

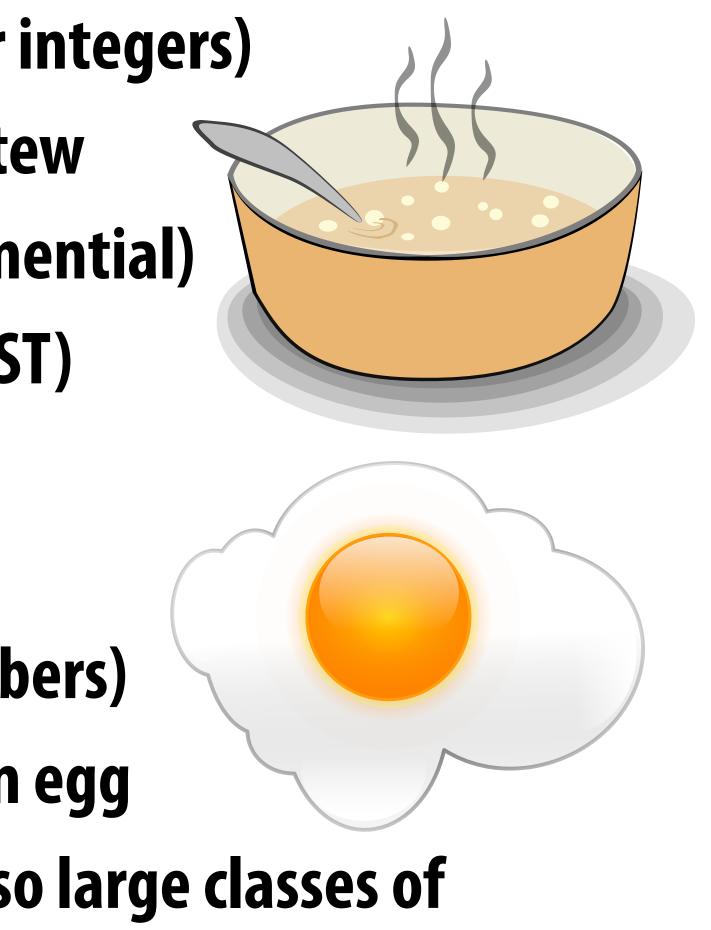


Nobuyuki Umetani, Yuki Koyama, Ryan Schmidt & Takeo Igarashi, *"Pteromys: Interactive Design and Optimization of Free-formed Free-flight Model Airplanes"*

Continuous vs. Discrete Optimization

DISCRETE:

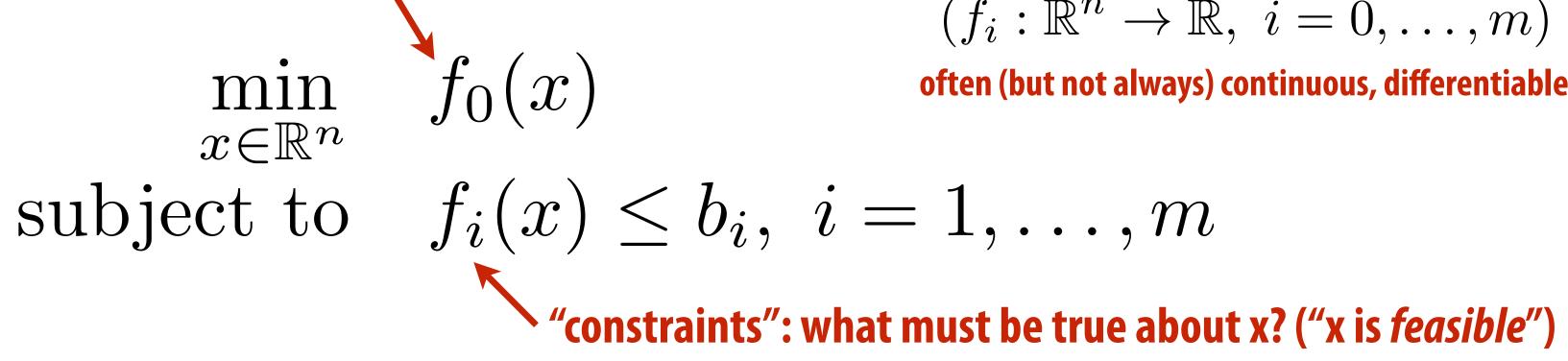
- domain is a discrete set (e.g., finite or integers)
- Example: best vegetable to put in a stew
 - Basic strategy? Try them all! (exponential)
 - sometimes clever strategy (e.g., MST)
 - more often, NP-hard (e.g., TSP)
- **CONTINUOUS:**
- domain is not discrete (e.g., real numbers)
- Example: best temperature to cook an egg
- still many (NP-)hard problems, but also large classes of "easy" problems (e.g., convex)



Optimization Problem in Standard Form

Can formulate most continuous optimization problems this way:

"objective": how much does solution x cost?



- **Optimal solution** x* has smallest value of f₀ among all feasible x
- Q: What if we want to *maximize* something instead?
- A: Just flip the sign of the objective!
 - Q: What if we want *equality* constraints, rather than inequalities?
- A: Include two constraints: $g(x) \le c$ and $g(x) \le -c$

 $(f_i : \mathbb{R}^n \to \mathbb{R}, i = 0, \dots, m)$

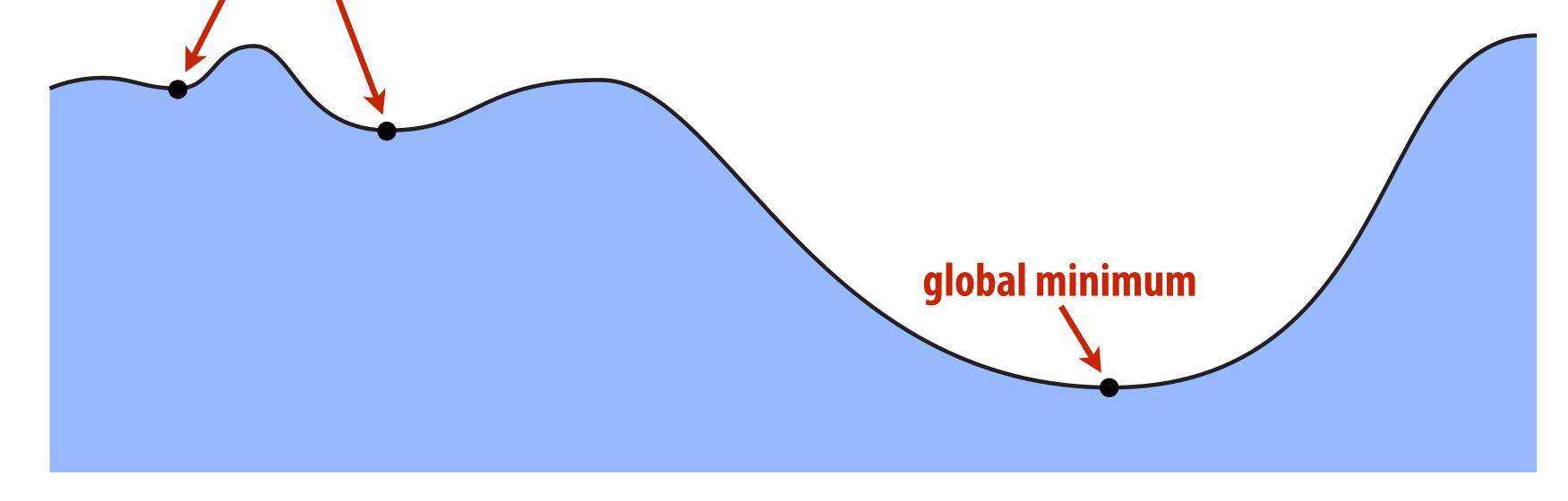
often (but not always) continuous, differentiable, ...

Local vs. Global Minima

local minima

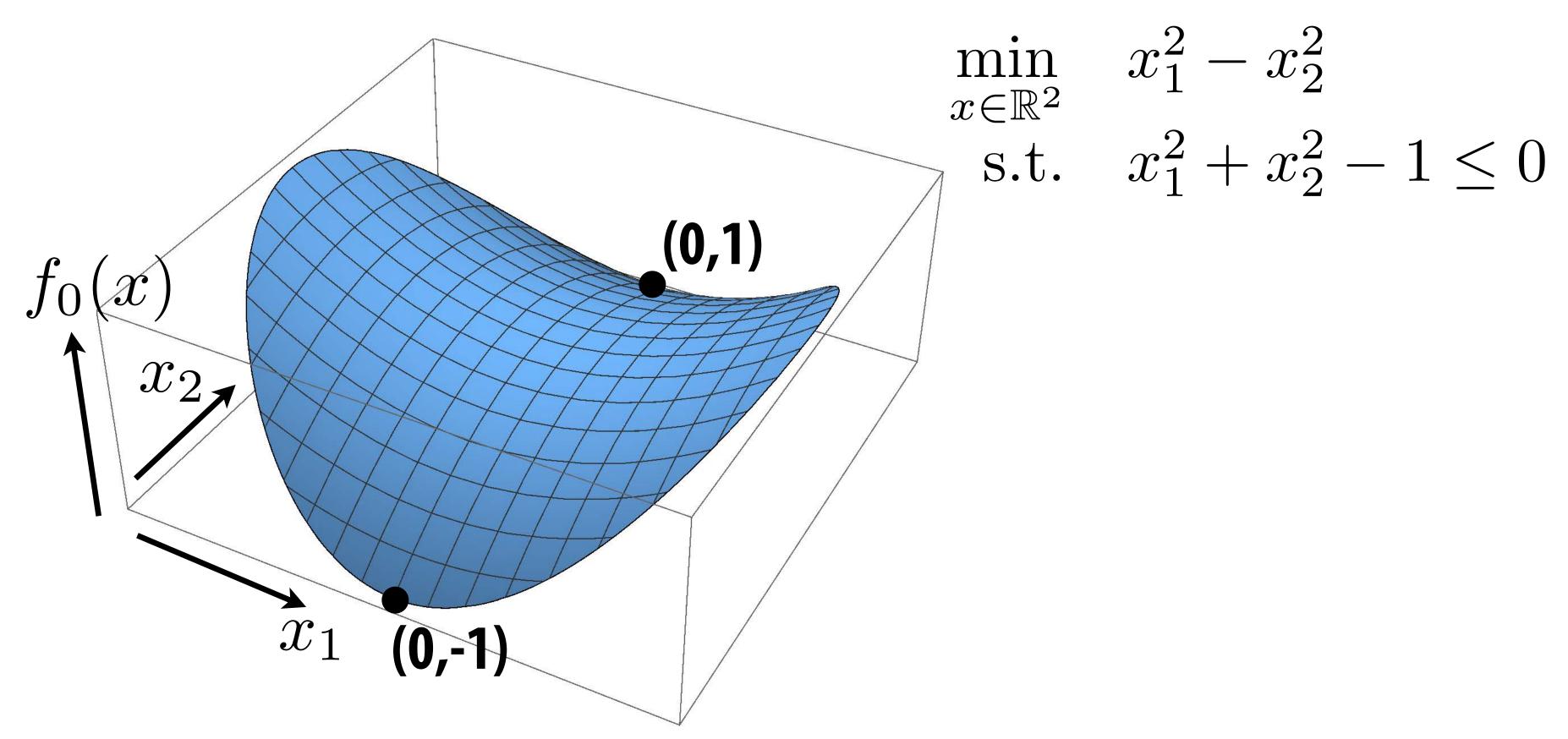
Global minimum is absolute best among all possibilities

Local minimum is best "among immediate neighbors"



Philosophical question: does a local minimum "solve" the problem? Depends on the problem! (E.g., real protein folding is *local* minimum) Other times, local minima can be really bad (e.g., path planning)

Optimization Problem, Visualized

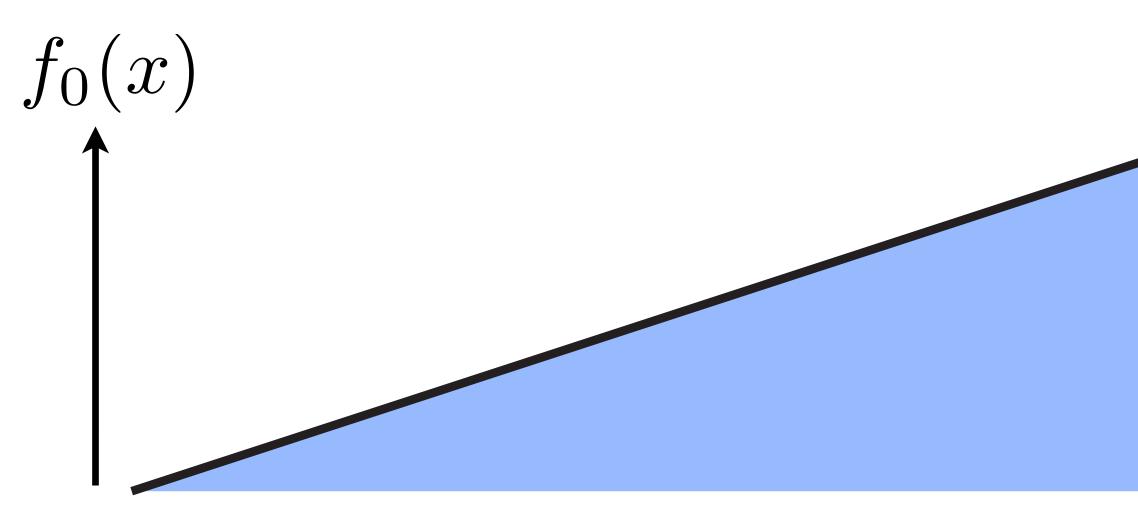


Q: Is this an optimization problem in standard form? Q: Where is the optimal solution?

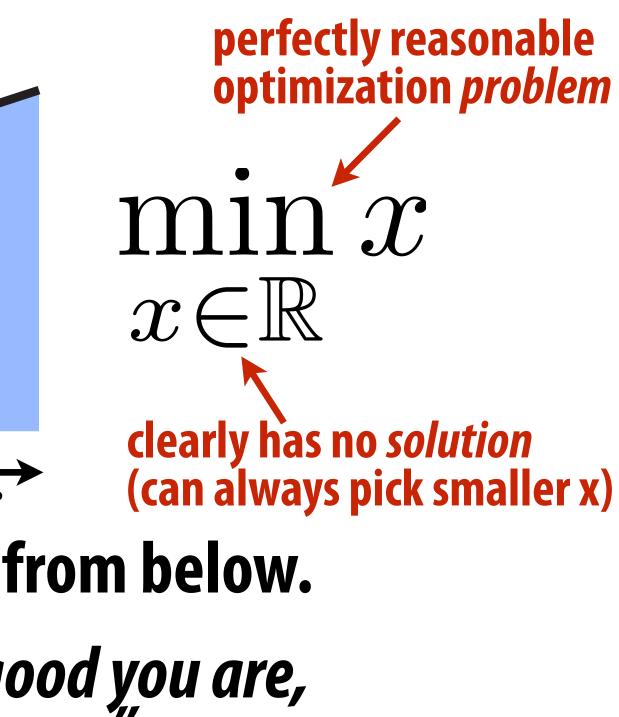
A: Yes. A: There are two, (0,1), (0,-1).

Existence & Uniqueness of Minimizers

- Already saw that (global) minimizer is not unique.
- **Does it always exist? Why?**
- Just consider all possibilities and take the smallest one, right?

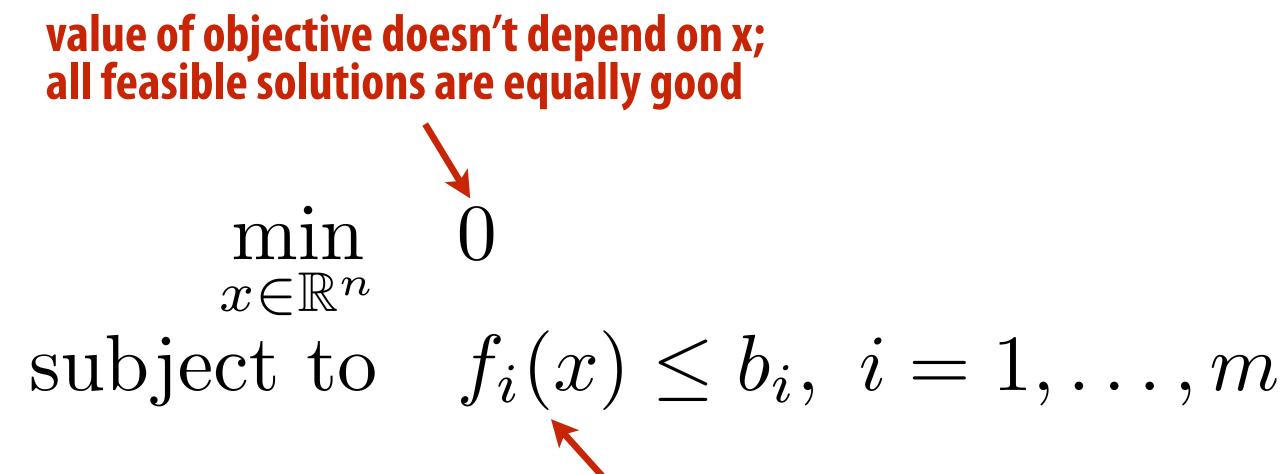


- $\mathcal{X}^{'}$ WRONG! Not all objectives are bounded from below.
- It's like that old adage: "no matter how good you are, there will always be someone better than you."



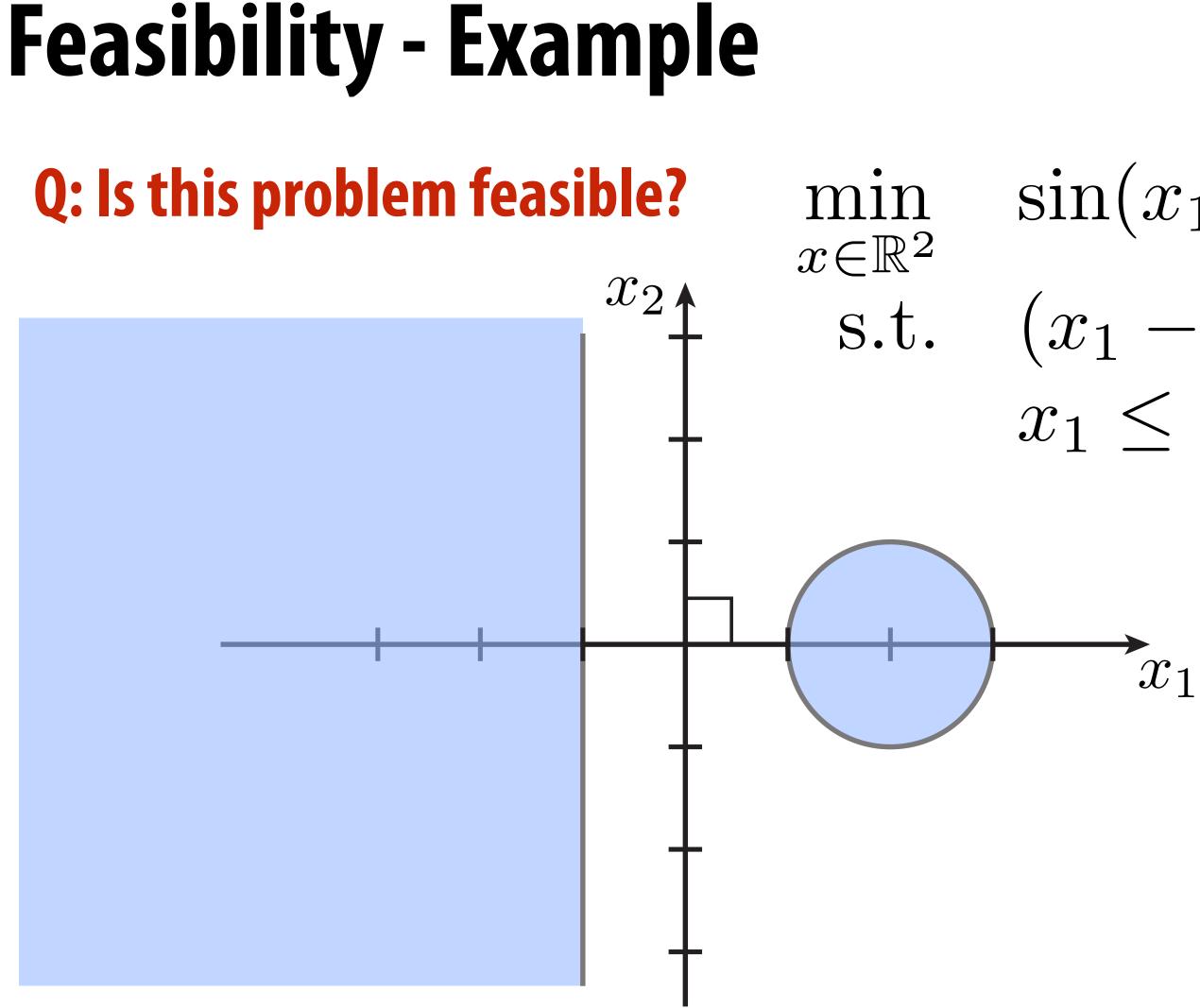
Feasibility

Ok, but suppose the objective is bounded from below. Then we can just take the best feasible solution, right?



- Not if there aren't any!
- **Every system of equations is an optimization problem.**
- But not all problems have solutions!
- (You'll appreciate this more as you get older.)

problem now is just finding a feasible solution which can be really hard (or impossible!)



A: No—the two sublevel sets (points where $f_i(x) \le 0$) have no common points, i.e., they do not overlap.

 $\sin(x_1) + x_2^2$ x $\in \mathbb{R}^2$ s.t. $(x_1 - 2)^2 + x_2^2 \le 1,$ $x_1 \le -1$

Existence & Uniqueness of Minimizers, cont. Even being bounded from below is not enough:

- Even being bounded from below is not e
 f(x)
- 0
- No matter how big x is, we never achieve the lower bound (0)
- So when does a solution exist? Two sufficient conditions:
- Extreme value theorem: continuous objective & compact domain
- Coercivity: objective goes to $+\infty$ as we travel (far) in any direction

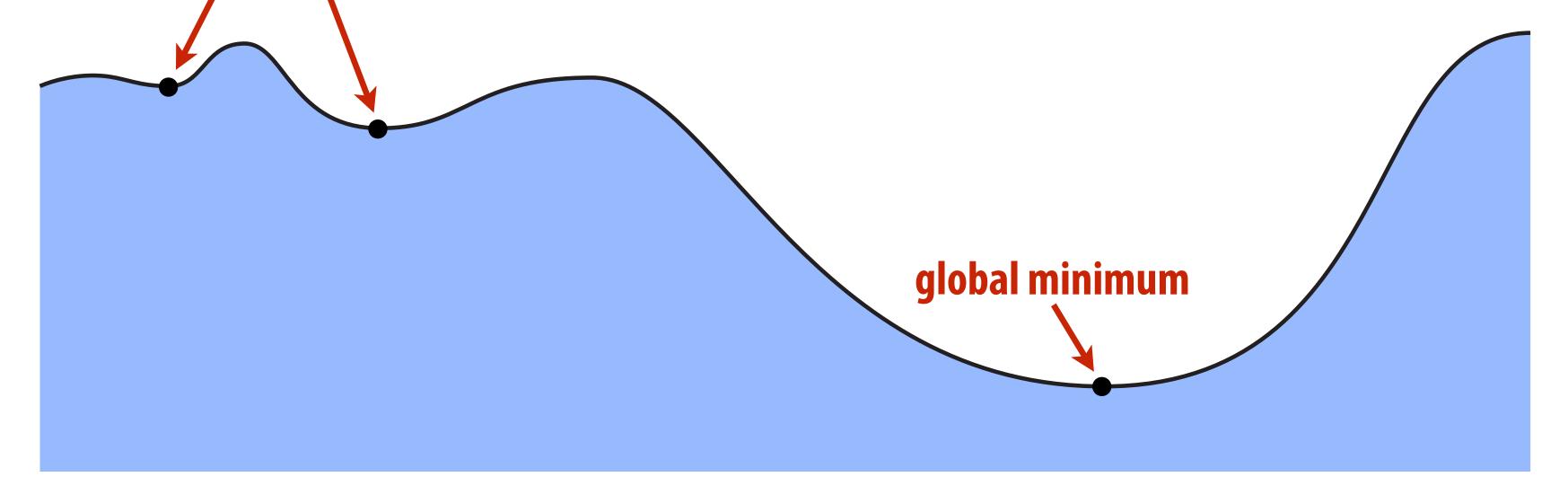
 $\min_{x \in \mathbb{R}} e^{-x}$

e the lower bound (0) *icient* conditions: ctive & compact domain ravel (far) in any direction

Characterization of Minimizers

- Ok, so we have some sense of when a minimizer might *exist*
- But how do we know a given point x is a minimizer?

local minima

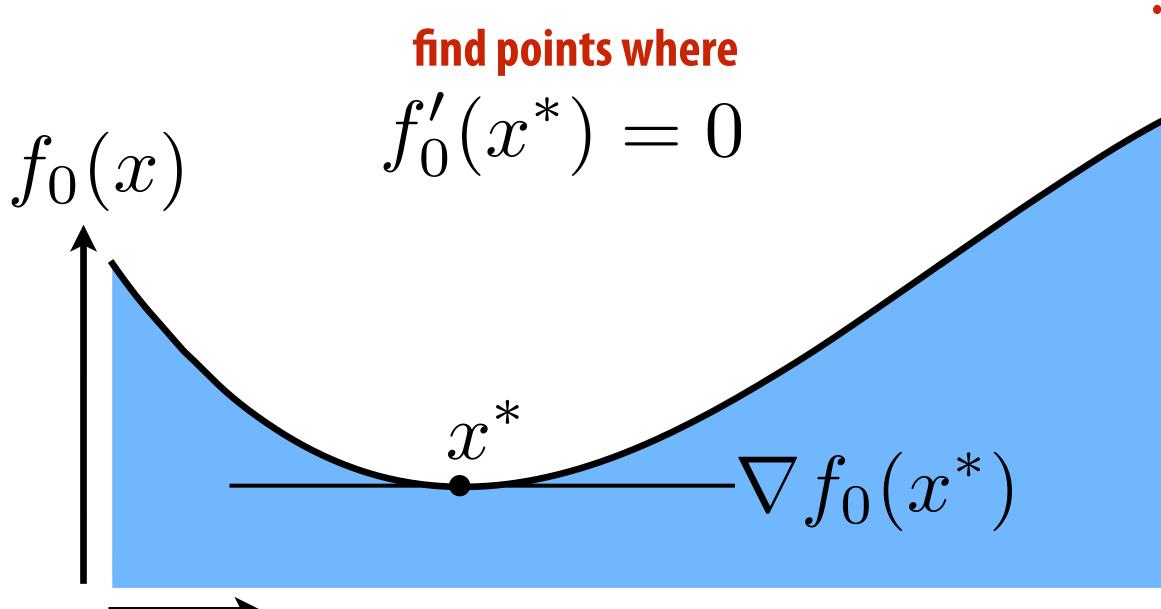


- Checking if a point is a global minimizer is (generally) hard
- But we can certainly test if a point is a local minimum (ideas?)
- (Note: a global minimum is also a local minimum!)



Characterization of Local Minima

Consider an objective $f_0: \mathbb{R} \rightarrow \mathbb{R}$. How do you find a minimum? (Hint: you may have memorized this formula in high school!)



- Also need to check *second* derivative (how?)
- Make sure it's *positive*

X

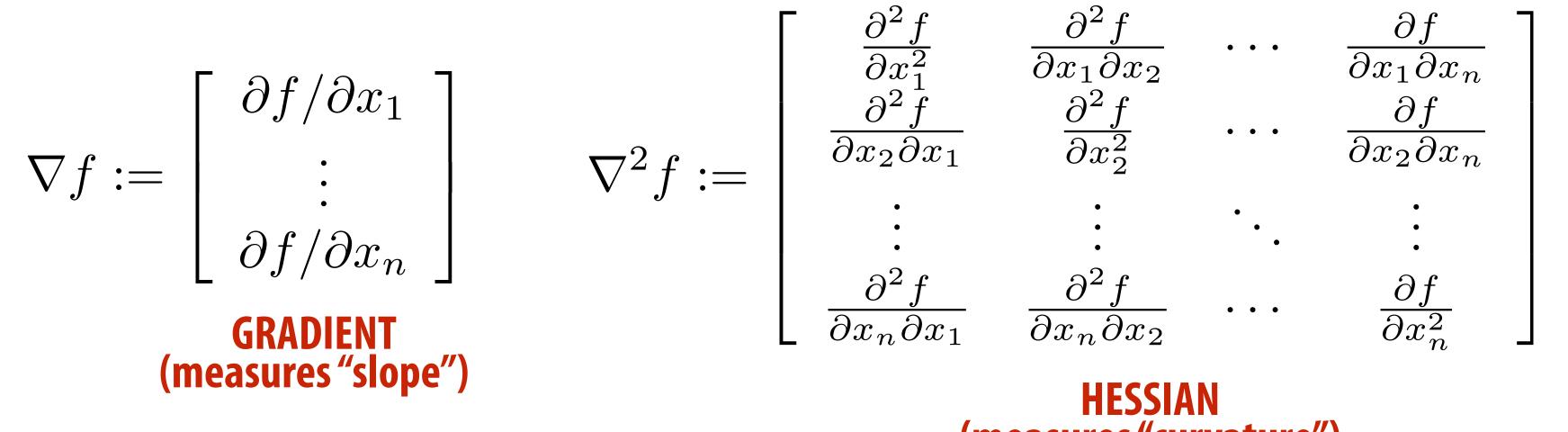
Ok, but what does this all mean for more general functions f_0 ?

...but what about this point?

must also satisfy $f_{0}''(x^{*}) > 0$

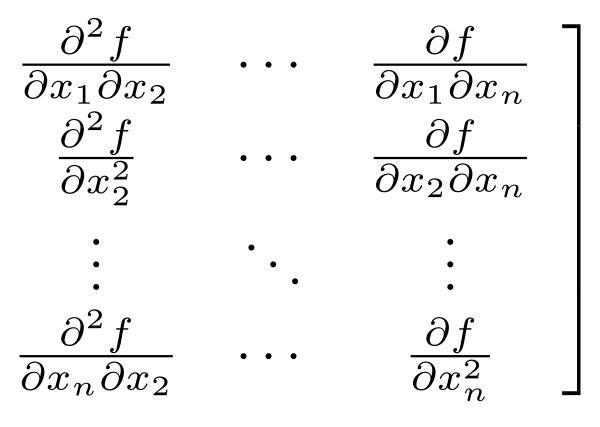
Optimality Conditions (Unconstrained)

- In general, our objective is $f_0: \mathbb{R}^n \to \mathbb{R}$
- How do we test for a local minimum?
- 1st derivative becomes gradient; 2nd derivative becomes Hessian



Optimality conditions?

$$\nabla f_0(x^*) = 0$$
1st order

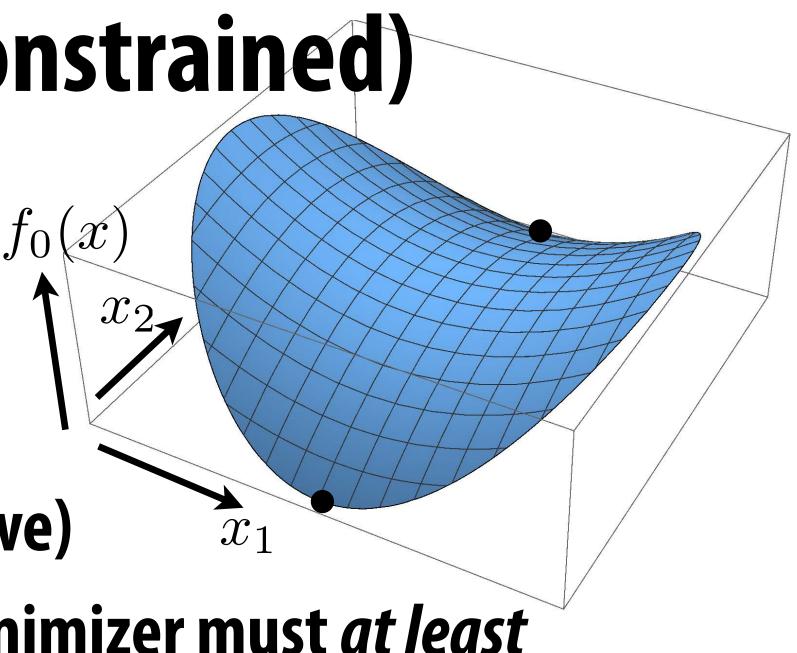


HESSIAN (measures "curvature")

 $\nabla^2 f_0(x^*) \succeq 0$ positive semidefinite (PSD) **2nd order**

Optimality Conditions (Constrained)

- What if we have constraints?
- Is gradient at minimizer still zero?
- **Is Hessian at minimizer still PSD?**



- Not necessarily! (See example above)
- In general, any (local or global) minimizer must *at least* satisfy the *Karush–Kuhn–Tucker* (*KKT*) conditions:

$$\exists \lambda_i \text{ s.t. } \nabla f_0(x^*) = -\sum_{i=1}^n \lambda_i \nabla f_i(x^*)$$
 sta

$$f_i(x^*) \le 0, \ i = 1, \dots, n$$
 pr

 \boldsymbol{n}

 $\lambda_i \geq 0, i = 1, \dots, n$ dual feasibility

$$\lambda_i f_i(x^*) = 0, \ i = 1, \dots, n$$

...we won't work with these in this class! (But good to know where to look.)

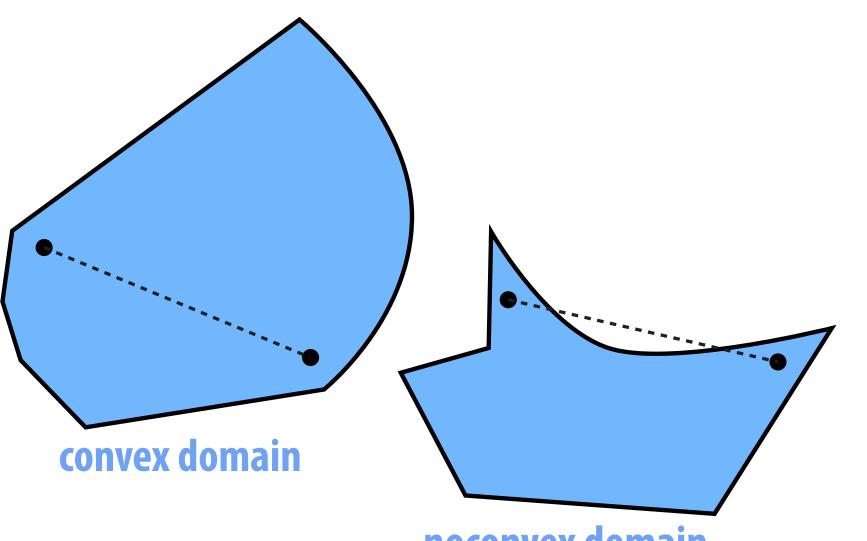
ationarity

imal feasibility

mplementary slackness

Convex Optimization

- Special class of problems that are almost always "easy" to solve (polynomial-time!)
- Problem *convex* if it has a convex domain *and* convex objective



noconvex domain

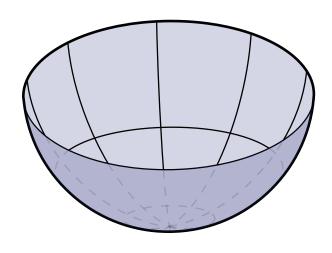
- Why care about convex problems in graphics?
 - can make guarantees about solution (always the best)
 - doesn't depend on initialization (strong convexity)
 - often quite efficient, but not always

f(x)nonconvex objective

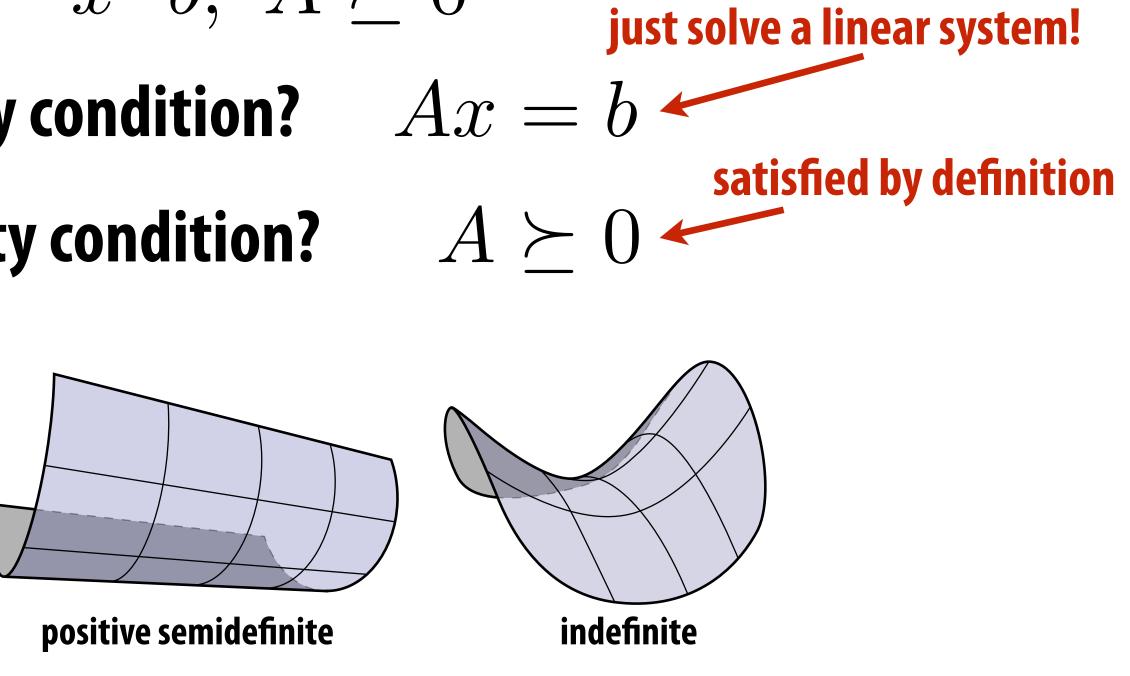


Convex Quadratic Objectives & Linear Systems

- Very important example: convex *quadratic* objective
- Already saw this with, e.g., quadric error simplification
- Valuable "variational" way of looking at many common equations
- Can be expressed via positive-semidefinite (PSD) matrix:
 - $f_0(x) = \frac{1}{2}x^{T}Ax x^{T}b, \ A \succeq 0$
 - **Q:** 1st-order optimality condition? Ax = b
 - Q: 2nd-order optimality condition?



positive definite



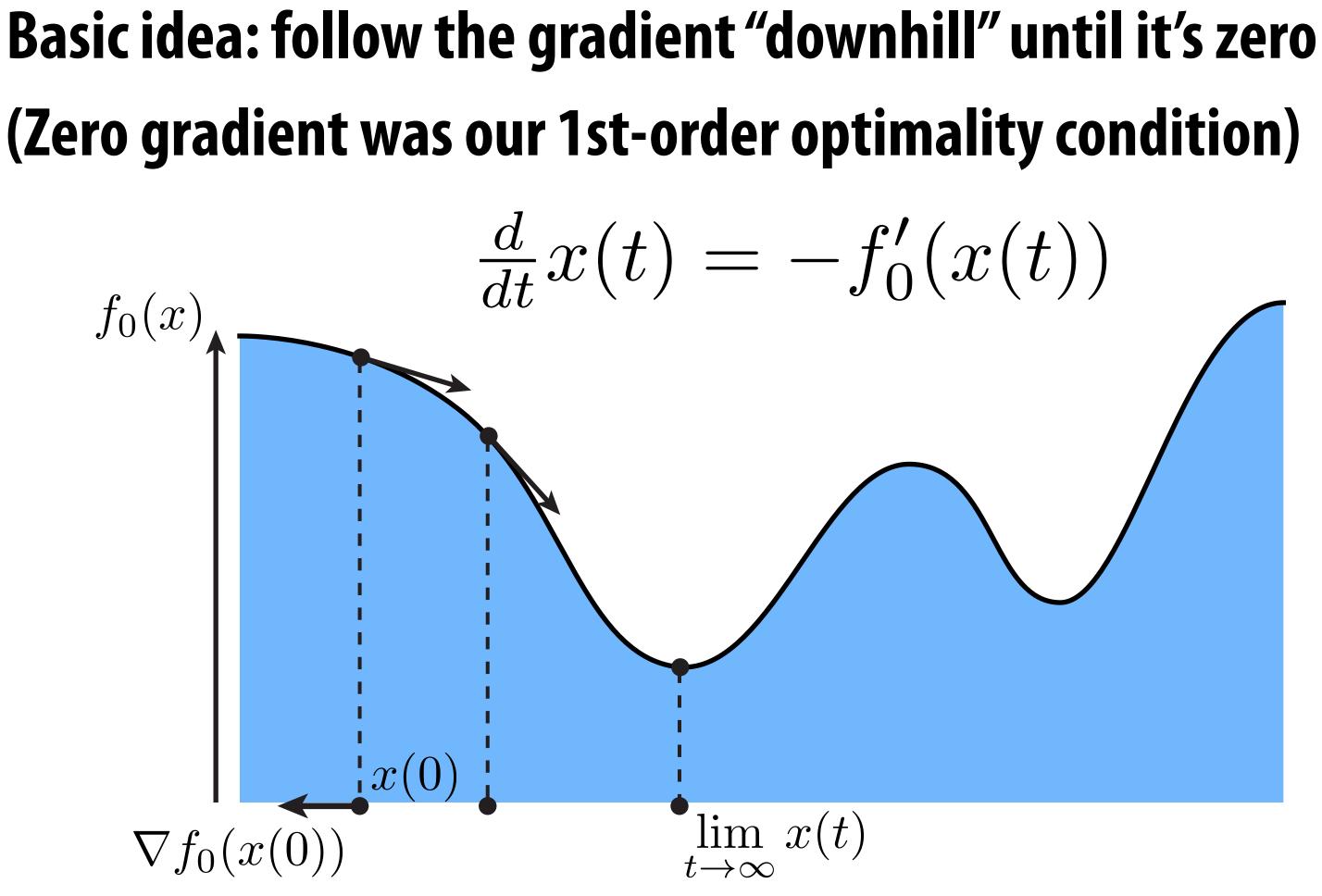
Sadly, life is not usually that easy. How do we solve optimization problems in general?

Descent Methods

An idea as old as the hills:



Gradient Descent (1D)



- Do we always end up at a (global) minimum?
- How do we compute gradient descent in practice?

Gradient Descent Algorithm (1D) Did you notice that gradient descent equation is an ODE? $\frac{d}{dt}x(t) = -f_0'(x(t))$ Q: How do we solve it numerically?

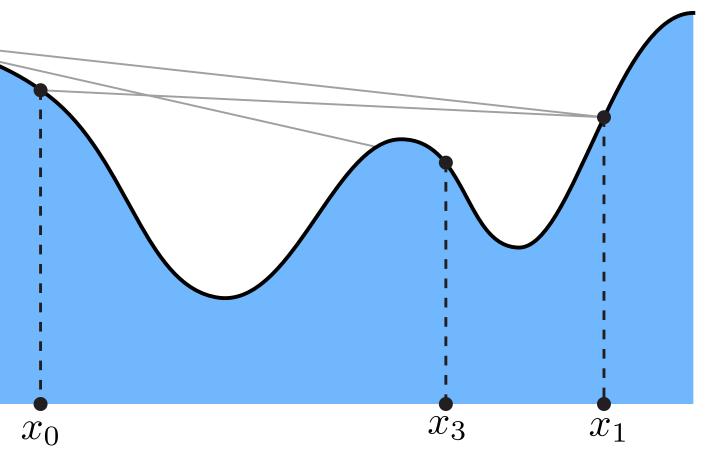
 $f_0(x)$

 x_2

- **One way: forward Euler:**

 $x_{k+1} = x_k + \tau f_0'(x_k)$

- Q: How do we pick the time step?
- If we're not careful, we'll go zipping all over the place; won't make any progress.
- Basic idea: use *"step control"* to determine step size based on value of objective & derivatives.
- A careful strategy (e.g., Armijo-Wolfe) can guarantee convergence at least to a *local* minimum.
- For now we will do something simpler: make τ really small!



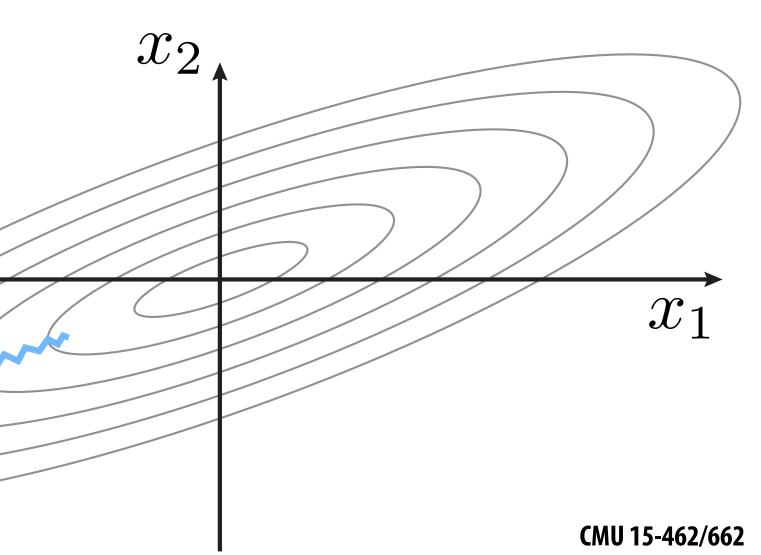
Gradient Descent Algorithm (nD)

- Q: How do we write gradient descent equation in general? $\frac{d}{dt}x(t) = -\nabla f_0(x(t))$
 - Q: What's the corresponding discrete update?

$$x_{k+1} = x_k - \tau \nabla j$$

- **Basic challenge in nD:**
 - solution can "oscillate"
 - takes many, many small steps
 - very slow to converge

 $f_0(x_k)$

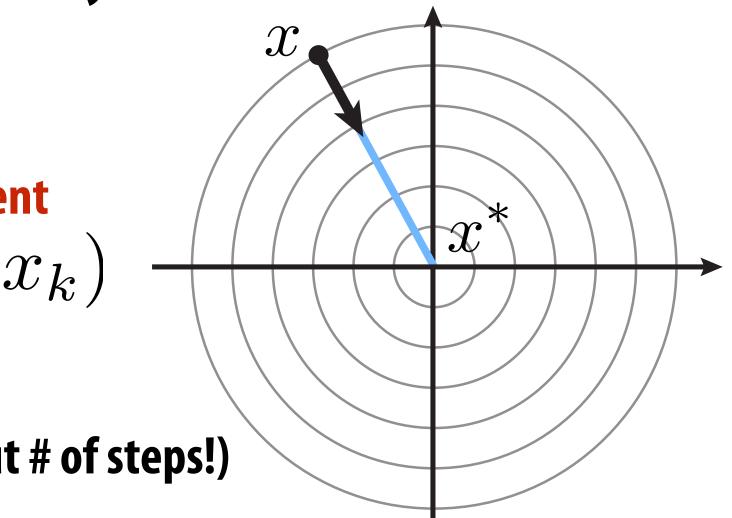


Higher Order Descent

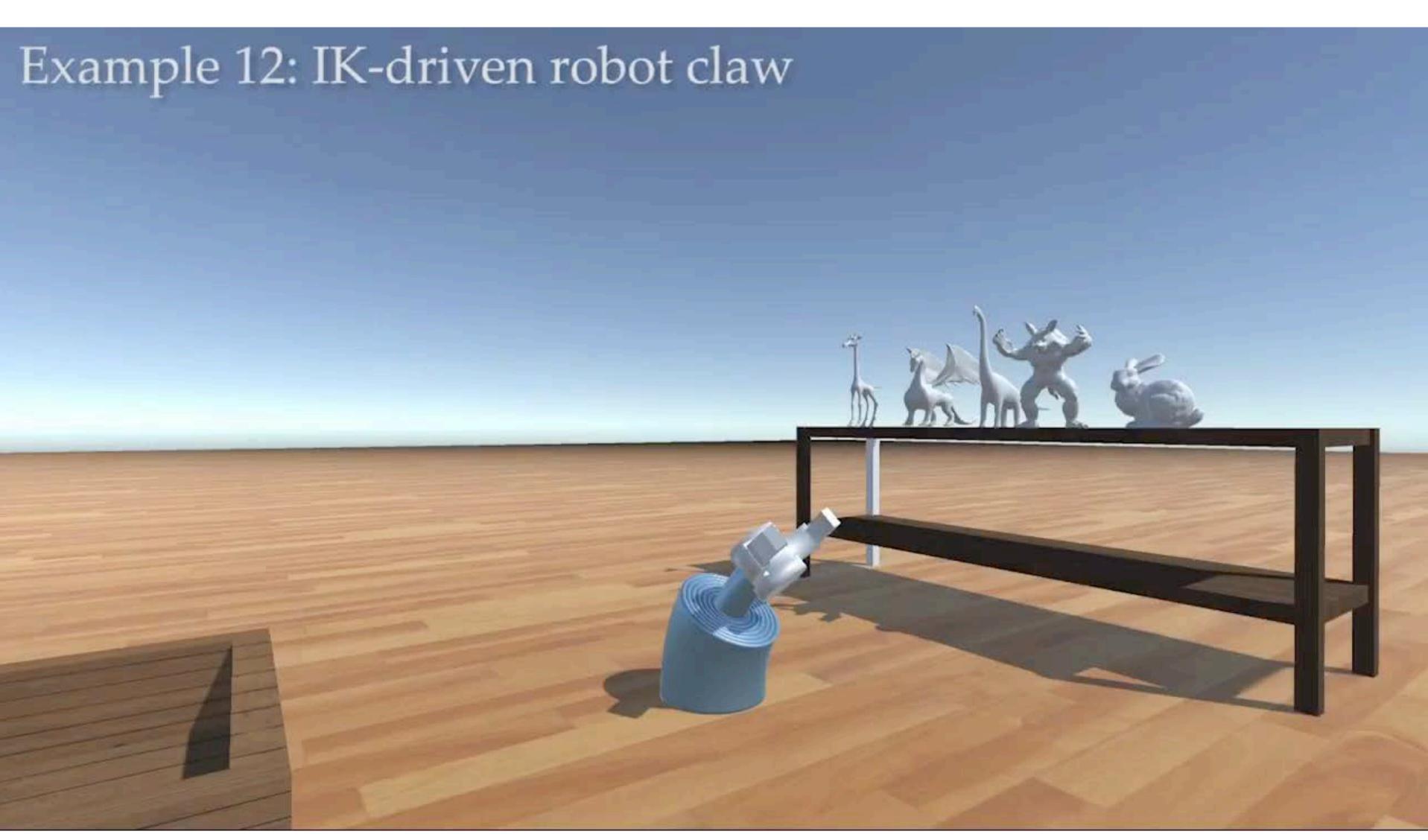
- General idea: apply a coordinate transformation so that the local energy landscape looks more like a "round bowl"
- Gradient now points directly toward nearby minimizer
- Most basic strategy: Newton's method:

$$\begin{aligned} \operatorname{gradie}_{k+1} &= x_k - \tau (\nabla^2 f_0(x_k))^{-1} \nabla f_0(x_k) \end{aligned}$$

- **Great for convex problems** (even proofs about # of steps!)
- For nonconvex problems, need to be more careful
- In general, nonconvex optimization is a BLACK ART
- Meta-strategy: try lots of solvers, see what works!
 - quasi-Newton, trust region, L-BFGS, ...



Example: Inverse Kinematics

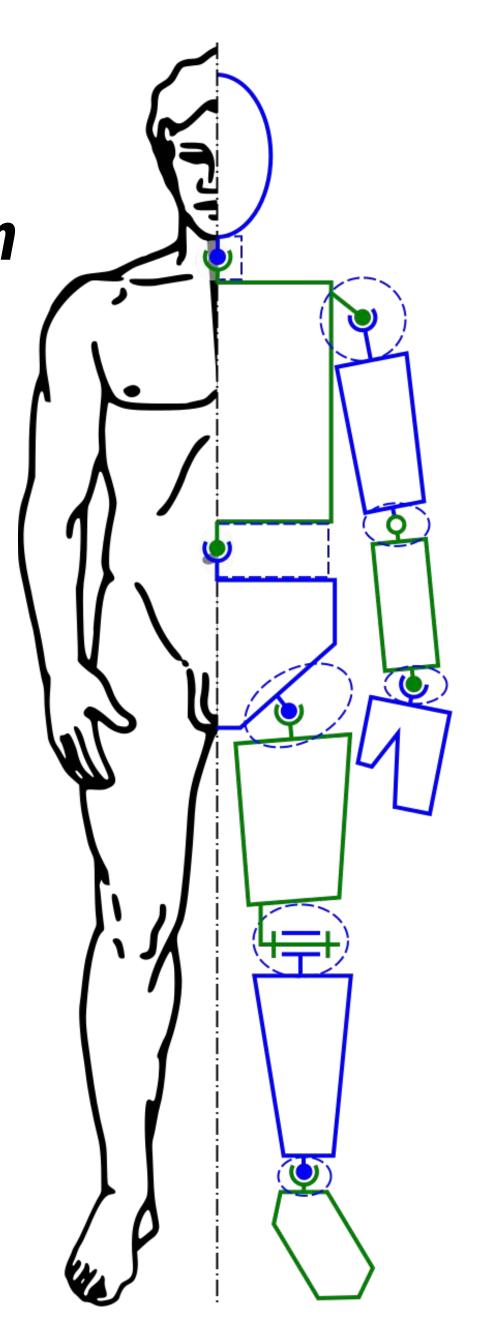


Forward Kinematics

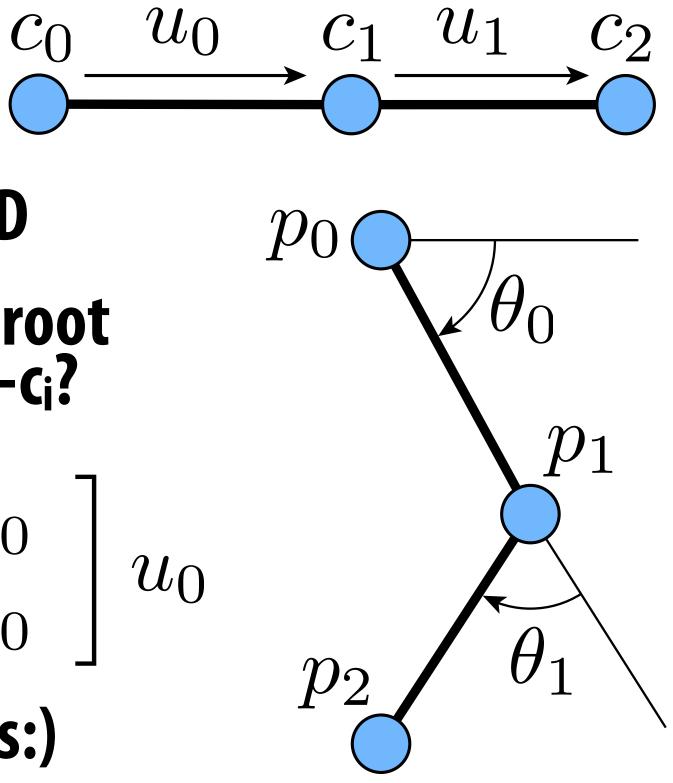
- Many systems well-described by a kinematic chain
- collection of rigid bodies, connected by joints
- joints have various behaviors (ball, piston, ...)
- also have constraints (e.g., range of angles)
- hierarchical structure (body \rightarrow leg \rightarrow foot)
- In animation, often called a rig
- How do we specify the configuration of a "rig"?
 - One way: artist sets each joint individually
 - Another way: ...optimization!

atic chair by joints ston, ...) ngles) foot)

a "rig"? |ually



Simple Kinematic Chain



- Consider a simple path-like chain in 2D
- Q: How do we write p₁ in terms of the root position p₀, angles, & vectors u := c_{i+1}-c_i?

$$p_1 = p_0 + \begin{bmatrix} \cos \theta_0 & \sin \theta_0 \\ -\sin \theta_0 & \cos \theta_0 \end{bmatrix}$$

For brevity, can use complex numbers:)

$$p_1 = p_0 + e^{i\theta_0} u_0$$

Q: How about p₂?

 $p_2 = p_0 + e^{i\theta_0}u_0 + e^{i\theta_0}e^{i\theta_1}u_1$

Simple IK Algorithm

Basic idea behind our IK algorithm:

- write down distance between final point and "target"
- compute gradient with respect to angles
- apply gradient descent
- **Objective**?

$$f_0(\theta) = \frac{1}{2} |\tilde{p}_n - p|$$

Constraints?

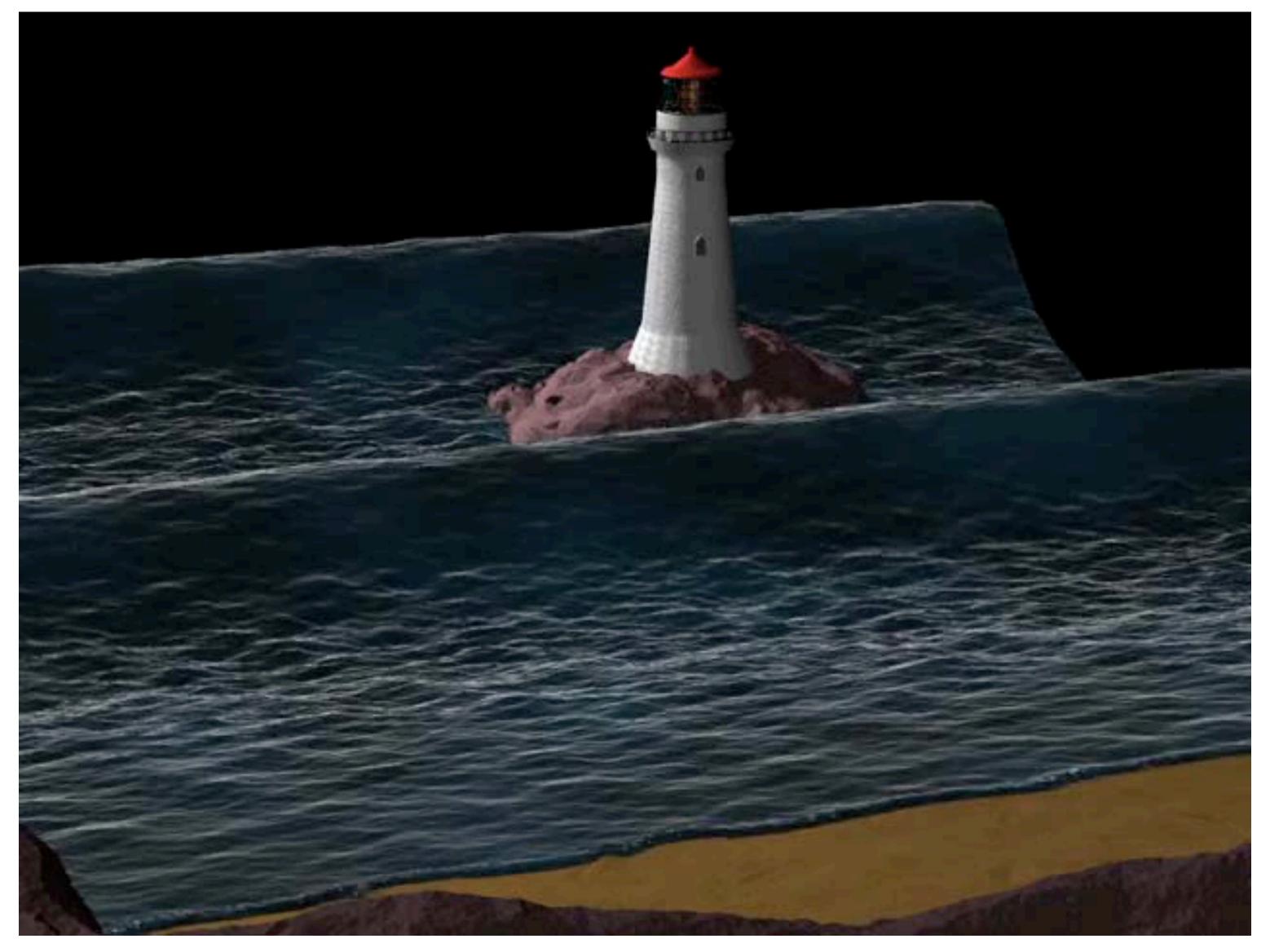
- None! The joint angle can take any value.
- Though we could limit joint angles (for instance)

pint and "target" gles

 $\mathcal{O}_n |^2$

alue. or instance)

Coming up next: PDEs in Computer Graphics



Frank Losasso, Jerry O. Talton, Nipun Kwatra, and Ron Fedkiw, "Two-Way Coupled SPH and Particle Level Set Fluid Simulation"